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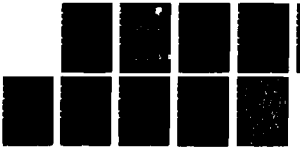

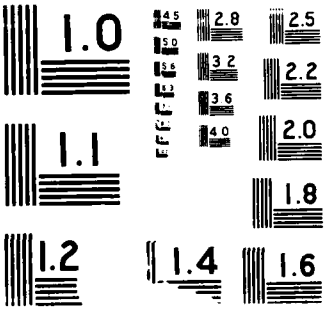
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COMPUTER SIMULATION OF ELECTROMIGRATION IN THIN FILMS

Rensselaer Polytechnic Institute

H. B. Huntington

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This report summarizes progress made toward computer simulation of the electromigration process in thin films. In particular it addresses the issues of forming a meaningful film, accounting for variations in the grain boundary energy and lattice mismatch, stress relaxations or annealing of the film, and mass flux within the film with and without a constraining overlayer. It incorporates vacancy concentration depended flux, but does not include the effects of void coalescence on the current density or temperature, and thus is an early life description.

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COMPUTER SIMULATION OF ELECTROMIGRATION IN THIN FILMS

The report describes an on-going effort to simulate actions which physically occur during the electromigration process. Important characteristics have been included such as diffusional processes which account for lattice mismatch angle or grain boundary energy, grain boundary energy equilibration or annealing, and the effects of an encapsulating layer. This description is meaningful in the early life of films when inhomogeneities of temperature and current density are not significant.

The author points out the formidable nature of extending this simulation to include the inhomogeneities which are characteristic of films near end of life. Further he indicates the range of time scales involved by solving for "semi steady state" solutions, because of the shortness of diffusional relaxation times as compared to film lifetimes. Future work in the area of Electromigration physics include improved descriptions of film growth to account for preferred grain boundary mismatch angles, and investigations of the quantum mechanical interactions of conducting electrons with point and extended defects such as dislocations.

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This report serves a double purpose. It is nominally the final report for the renewal project under USAF contract number F-30602-81-C-0193 RADC Task No. N-6-5754 but it also serves to review the progress made during some fourteen months under contract SCEEE-PDP/85-0051 as well as the contract just completed. The report is divided into four sections. The first, or introduction, treats quite briefly the principal background based on earlier work preceeding the SCEEE contracts. The second section recounts some of the complications inherent in the process of equilibrating grain boundary tensions and how they have recently been resolved. Section three deals with electromigration under a free surface and section four is concerned with the more complex situation resulting from electromigration under a passivating film. Finally we discuss briefly what the succeeding program for this investigation might be.

I. Review of Earlier Work

The purpose of this simulation is to develop a representation of the actions that physically occur in a stripe during the period of early deterioration and to explore the influence of various factors in stripe environment, specifically stripe annealing and stripe passivation by a constraining surface film.

At this point we review briefly the results of earlier work, preceding the SCEEE contracts. The first step was to develop a program that would generate randomly a reasonable network of grain boundaries for a stripe of adjustible dimensions. For this an extended Voronoi program was applied. Next the vertices of the network were allowed to relax to attempt to equilibrate the grain boundary stresses as it was believed that the surface tensions at the grain boundaries were closely linked to the respective diffusivities and that their equilibrium at the vertices would tend to reduce

the matter build-up or reduction with time. This action, as a form of annealing, should tend to increase stripe lifetime.

With the stripe network in place the mass motion induced by electromigration was introduced through the appropriate diffusion equation modified by the addition of a driving term. It was apparent from the values invoked by this equation that the time constants were very short compared with stripe lifetimes and that one must deal almost exclusively with the "semi-steady state" solutions in calculating the mass transfer. The cases of the free surface and surface constrained by passivating layers were considered separately.

II. Finalizing Stress Equilibrium

During the present period more work was done on implementing the stress equilibrium which had been left in an unfinished state earlier. Although the concept of allowing the network vertices to move to relax the unbalanced grain boundary stresses is simple, the process of implementation is fraught with all the difficulties associated with finding a minimum of a function of a large number of coordinates. In this case it was not necessary to set all net stresses to zero but only reduce them to below a certain level. Difficulty in particular occurred when stress was in a certain grain boundary segment strong enough to pull together the segment's end vertices. The shortened segment complicated the equilibrium process and required the establishment of carefully considered criteria for coalescence. After coalescence there was still the possibility that the combined vertex would separate again into two vertices creating a new segment roughly orthogonal to the original segment; the treatment had to be programmed to explore this possibility. Finally one had to allow for the disappearance of any triangular grain which lost a side through coalescence.

All these considerations complicated the equilibrium program but were eventually mastered.

III. Mass Motion; Free Surface

After setting up the grain boundary network and incorporating the annealing of the grain boundary tension, the action of forces during mass transport was investigated. The basic equation for the number of atoms per unit length of grain boundaries $M_\sigma(x,z,t)$, in stripe numbered σ is

$$\frac{\partial M_\sigma}{\partial t} = D_{\perp\sigma}\left[\frac{\partial^2 M_\sigma}{\partial x^2} - A_\sigma \frac{\partial M_\sigma}{\partial x}\right] + D_{||\sigma} \frac{\partial^2 M_\sigma}{\partial z^2} \qquad (1)$$

Here $D_{\perp\sigma}$ and $D_{||\sigma}$ are the diffusion constants perpendicular and parallel to the dislocations that make up small angle grain boundaries in the network, i.e. respectively parallel and perpendicular to the surface of the substrate. The quantity A_σ relates to the electromigration drive and equals $|e|E \cos \phi\ Z^*/kT$, where Z^* is the effective charge number, a dimensionless quantity which measures the strength of the electromigration force and ϕ is the angle which the grain boundary makes with the current. The boundary conditions for the solution of the mass flow equation is that the flux, given by $D_{\perp\sigma}(A_\sigma M_\sigma(x) - \frac{\partial M_\sigma(x)}{\partial x})$ vanish at the vertices that accumulate material at the ends of the segment in question. On the other hand the deficit vertices (those from which material is taken away) are assumed to develop voids, which can be considered most simply as empty circular cylinders going from surface

to substrate. The boundary condition here then are that m(x,t) be zero where we take

$$M(x,t) = M_o + m(x,t) \tag{2}$$

Here M_o is the equilibrium number of atoms per unit length in the grain boundary,

$$M_o = N\, d\, \delta \tag{3}$$

where N is the number of atoms per unit volume, d is the thickness of the stripe and δ is the width of the grain boundary taken nominally to be 3×10^{-8} cm. Undoubtedly the concept of a circularly symmetric void is an oversimplification. At one time we considered that the missing material appeared as grooves down the grain boundaries but more careful consideration indicated that the surface driving forces would strongly favor the voids, although they are probably somewhat irregular.

Straight numerical solution of eq. (1) encounters serious convergence problems. Recourse to analytical approximations soon shows that the natural time constants are far too short to be useful. If the typical segment length is L, then $L^2/D_\perp$ is of the order of an hour as compared to stripe lifetimes of months. Apparently one can afford to disregard the transients and move to what we have called "semi-steady state" solutions.

In this section the case of deterioration at a free surface will be considered. Excess material will flow unimpeded up through the grain

boundaries and spread nearly uniformly over the surface creating hillocks of low contour. The matter concentration in the grain boundaries will be strictly time independent and of the form,

$$m(\bar{r}) = m(x)\ (\pi/2d)\ \cos\ (\pi z/2d) \tag{4}$$

where z is measured from the substrate. The function m(x) satisfies the equation,

$$m''(x) - A_\sigma\, m'(x) = (D_{||}/D_\perp)\ \left(\frac{\pi}{2d}\right)^2\ m(x), \tag{5}$$

which has solutions of the form $a_1\ e^{\gamma_1 x} + a_2\ e^{\gamma_2 x}$, where

$$\gamma_{1,2} = \frac{A}{2} \pm \left[(D_{||}/D_\perp)(\pi/2d)^2 + \left(\frac{A}{2}\right)^2\right]^{1/2} \tag{6}$$

However it turns out that in most cases $A/2 < (D_{11}/D_1)\ (\pi/2d)^2$ and, in the interest of simplifying the simulation, the A has been dropped or

$$\gamma_{1,2} = \pm\ (D_{11}/D_1)^{1/2}\ (\pi/2d) \tag{6a}$$

Another way to see that this approximation is reasonable to look at the boundary condition at the vertices, for the flux, $D_{\perp\sigma}(A_\sigma M_\sigma(x) - m_\sigma'(x)$. Initially the $M_\sigma(x)$ is a constant and the summation, $F_v = \sum A_\sigma D_{\perp\sigma} M_o$ is positive at the excess vertices and negative at the deficit vertices. Since $m(x) << M_o$ it is reasonable to drop the term $A_\sigma\ m(x)$. At the excess vertices one has then $F_v = |\sum_\sigma D_{\perp\sigma} m_\sigma'(x)|$.

It is useful to designate the class of segment by the nature of its

bounding vertices: + + for those with excess vertices at each end, + - for those with an excess at one end and a deficit vertex at the other, and - - for those bounded by two deficit vertices. For the + + segments the m(x) is given by the the sum of two exponentials. For the + - segments a sinh function appears and for the - - segments m(x) vanishes. At the deficit vertices F_v gives approximately the time rate of increase of the void cylinders. There is, however, a small correction from "spill-over" from the + - segments. Since the sinh has a non-vanishing derivative for zero argument, there will be some outward diffusional flow (usually small) from these segments.

There is a universal problem in all this simulation in determining how to divide F_v into tne respective f_σ that flow into tne individual segments. The exact result would require the solution of a large set of interrelated linear equations. Rather than get involved in this complication we have chosen to move by successive approximations. Basically $f_i = D_{\perp i}|\frac{\partial m_{vi}}{\partial x}|$. The m_{vi} are, however, independent of i. One can not evaluate the derivative without knowing the form of $m_\sigma(x)$ but one guesses that it can be approximated by m_v/λ_i. Here the parameter λ_i is set equal the shorter of L_i, the length of the ith segment, and the parameter $(D_\perp/D_{||})^{1/2}$ $(2d/\pi)$. Refinement of this approximation can proceed by iteration. Next one determines the m_v as equal to $F_v/\sum_i D_{\perp i}/\lambda_i$ (see progress report #3 p. 4) and hence m(x) everywhere.

The end result of these simulations can be presented pictorially. For this we show the network at a particular instant in time with scaled circles around the deficit vertices and graded cross-hatching on the + + and + - segments. The cross-hatching represents the matter concentration in the grain

boundaries and as such does not change (after a brief transient period which we pass over); the areas of the circles will increase linearly with time. This situation will hold throughout the period of initial damage and will only change when the temperature distribution in the stripe changes because of inhomogeneities in the current distribution caused by the presence of the voids.

IV. Mass Motion; Passivated Surface

In this section we consider the effect of the presence of a passivating layer constraining the outflow of material from the grain boundaries. Mathematically this is a bit more complex, since now the concentration of matter in the grain boundaries is building up with time. Again we disregard any transients and look for "semi-steady state" solutions of the mass flow equation. There are two: $m(x) = hx$ and $m(x,t) = k\,x^2 + 2kt$. For the + -segments only the first is applicable corresponding to a situation where matter flows uniformly down the segment with no change in concentration with time. For the ++ segments both forms are needed,

$$m_\sigma(x) = k_\sigma x^2 + 2D_{1\sigma}\, k_\sigma t + h_\sigma x. \tag{5}$$

We take the incoming flux at the left and right vertices of the segment to be given by

$$f_{L/R} = D_{1\sigma}\,(k_\sigma L_\sigma \mp h_\sigma), \tag{6}$$

where the origin for x is put at the center of the segment of length L_σ.

Since $m_{L/R} = k_\sigma (L_\sigma/2)^2 + 2D_\sigma k_\sigma t \mp h_\sigma L_\sigma/2$, (7)

it follows that

$$h_\sigma = (m_R - m_L)/L_\sigma \tag{8}$$

$$k_\sigma = (f_L + f_R)/2D_{\perp\sigma} L_\sigma \tag{9}$$

A. Initial Approximate Solution

Again one faces the problem of avoiding the solution of a large simultaneous system of linear equations. We have chosen to take eq. (5) and drop the h_σ term to get an approximate expression for k_σ in terms of m_σ,

$$k_\sigma = m_v \left[(L/2)^2 + 2D_{\perp\sigma} t\right]^{-1} \tag{10}$$

By substituting the approximate expression for k_σ one into eq. (6) obtains

$$f_{v\sigma}/m_v = L \frac{D_{\perp\sigma}}{(\frac{L}{2})^2 + 2tD_{\perp\sigma}} \tag{11}$$

So much for the (+ +) segments. Returning now to the (+ -) segments we have (3rd progress report p. 6)

$$f_\sigma = D_\perp m_v/L_\sigma + \frac{1}{2} L_\sigma \frac{dm_v}{dt} \tag{12}$$

The first term accounts for the straight-through flow from + vertex to - vertex. The second term gives the mass build-up in the segment that comes with the steepening of the slope m_v/L_σ. Combining we have

$$F_v = \sum f_\sigma = \sum_\sigma^{+\,+} D_{\perp\sigma} L_\sigma \left[(\frac{L}{2})^2 + 2 D_{\perp\sigma} t\right]^{-1} m_v \tag{13}$$

$$+ \sum_\sigma^{+\,-} \{D_{\perp\sigma} m_v/L_\sigma + \frac{1}{2} L \frac{dm_v}{dt}\}$$

The evaluation of m_v in terms of the known F_v is straightforward if the vertex connects only (+ +) segments or only (+ −) segments:

a) Only (+ +) segments

$$m_v = F_v \left[\sum^{+\,+} D_{\perp\sigma} L_\sigma \left[\left(\frac{L_\sigma}{2}\right)^2 + 2\, D_{\perp\sigma} t \right]^{-1} \right]^{-1} \tag{14a}$$

which indicates an m_v that increases steadily with time as long as all segments stay (+ +).

b) Only (+ −) segments

$$m_v = F_v \left[\sum^{+\,-} (D_{\perp\sigma}/L_\sigma) \right]^{-1} \{1-\exp-\sum^{+\,-} (2D_{\perp\sigma} t/L_\sigma)/(\sum^{+\,-} L_\sigma)\} \tag{14b}$$

For segments of modest length the transient will probably be short lived and m_v soon reaches its saturation value of $F\left[\sum^{+\,-} (D_{\perp\sigma}/L_\sigma) \right]^{-1}$.

c) The equation (13) is not simple to integrate if both (+ +) and (+ −) segments are involved but it appears that again m_v will saturate in time so that $\frac{dm}{dt}$ can be considered small after an early transient. On this basis we take $m_v = m_{v1} - m_{v2}$ where

$$m_{v1} = F_v \left[\sum^{+\,+} L_\sigma \; D_{\perp\sigma} \left(2D_{\perp\sigma} t + \left(\frac{L_\sigma}{2}\right)^2\right)^{-1} + \sum^{+\,-} (D_{\perp\sigma}/L_\sigma) \right]^{-1} \tag{15}$$

Let us abbreviate the $[\quad]$ by $\pi_v(t)$. Then

$$m_{v1} = F_v/\pi_v(t) \tag{15a}$$

and $$F_v = m_v \pi_v(t) + \left(\sum^{+\,-} \frac{1}{2} L_\sigma\right) \frac{dm_v}{dt} \tag{13a}$$

Since the final term is small we approximate $\frac{dm_v}{dt} = \frac{dm_{v1}}{dt}$

$$\frac{dm_{v1}}{dt} = -\frac{F}{\pi}\frac{d\pi}{dt} = F\pi^{-2} \sum_{2}^{++} L_\sigma D_{\perp\sigma}^2 \left[2D_{\perp\sigma}t + \left(\frac{L_\sigma}{2}\right)^2\right]^{-2} \tag{16}$$

$$\text{Next } m_{v2} = \frac{F}{4\pi^3}\left[\left(\sum^{+-}\left(\frac{L_\sigma}{2}\right)\right)\left(\sum^{++}\left(\frac{L_\sigma}{2}\right)\right)\left(t + \left(\frac{L_\sigma}{2}\right)^2 \frac{1}{2D_{\perp\sigma}}\right)^{-2}\right] \tag{17}$$

Hopefully (17) is a small correction term.

B. Refinement by Iterations

Next one pursues an iteration procedure to refine on the approximation of dropping h at eq. 11. From the equations (15) and (17) one knows m_v in terms of F_v, L_σ, and $D_{\perp\sigma}$. From the $m_{L/R}$ one determines h_σ from eq. (8) and new (first) values of k_σ from eq. (10). From k_σ and h_σ the new $f'_{v\sigma}$ can be obtained for the (+ +) segments via eq. 6. For the (+ −) segments one uses eq. 12. Since $\frac{dm_{v2}}{dt}$ is assumed small, it is probably adequate to approximate it from eq. 16. Next one applies the condition $\sum_\sigma f_{v\sigma} = F_v$, a known quantity. Since the new $f_{v\sigma}$'s do not automatically satisfy $\sum f_\sigma = F_v$ and are indeed proportional to m_v, it is logical to renormalize to new $m_v \to m'_v$.

$$m'_v = m_v \frac{F_v}{\sum_\sigma f'_{v\sigma}} \tag{18}$$

With the new m'_v one is ready for a second round in the iteration process.

Brief mention is here made of the changes that occur at the deficit vertices. The $F_v < 0$ continue steadily to enlarge the voids but one must also look to the spill-over terms which tend to fill them up as discussed in the fourth progress report. Here the spill-over can be expressed

$$S - 0 = \sum_\sigma^{-+} D_{\perp\sigma}\, t\, m_{v+}/L_\sigma \tag{19}$$

Eventually this term could exceed F_v and in due course fill up the void changing the vertex from - to +.

Perhaps the simplest way to check on the progress toward convergence in the iteration process is to present the results graphically and inspect the superimposed transparent representations of successive steps in the iteration.

C. Time steps

After determining the m values throughout the network at a time sufficiently short to avoid non-linear effects from saturation and spill-over, the program must be extended through subsequent time intervals to trace the mass motions. Our procedure is to start with equation (13a) as it holds at two different times t_1 and $t_2 = t_1 + \Delta t$. Since F is quite time independent it drops out on subtraction and we have our relation for the finite difference of m, or $\Delta m = m(t_2) - m(t_1)$:

$$-\Delta m_v = \left[m_v(t_1)\Delta\pi + \left(\sum^{+-} \frac{L_\sigma}{2}\right)\left\{\left(\frac{dm_v}{dt}\right)_{t_2} - \left(\frac{dm_v}{dt}\right)_{t_1}\right\}\right]/\pi(t_2) \qquad (20)$$

There are simplifications for two special cases:

a) If the + vertex links only to - vertices, then there is no change in m_v unless t_1 lies in the transient region.

b) If the + vertex links only to + vertices, then there is no term involving $\frac{dm_v}{dt}$.

c) If both + and - vertices are involved, we proceed by considering the derivative terms as small,

$$-\Delta m_{v1} = \frac{m_v(t_1)\ \Delta\pi}{\pi(t_2)} \tag{21a}$$

$$-\Delta m_v \simeq -\Delta m_v + \pi(t_2)^{-1}\left(\sum^{+,-} \frac{L\sigma}{2}\right)\left\{\frac{\Delta m_{v1}}{\Delta t} - \frac{m_v\ (t_1)}{t_1}\right\} \tag{21b}$$

Once the Δm_v and consequently $m_v(t_2)$ are determined, one can proceed to establish the new h_σ and k_σ and to calculate the additional spill-over in Δt.

With successive time steps the growth of m_v will saturate eventually, even for vertices with only + neighbors.

V. Continuing Program

Fortunately we have some support from an industrial company to continue somewhat longer our investigation of this simulation. We plan to implement with a program calculation the analysis for the passivated surface described in part 4 and to compare results with those for the free surface using both unannealed and equilibrated networks. Rupture of the passivating layer at m greater than a certain critical value, m_c, should also be considered.

We plan to introduce the effects of surface electromigration in inducing void motion.

In the long term an effort should be made to consider the influence of temperature and current inhomogeneities caused by the presence of the voids although this is a formidable complication.

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